Towards heavy-mass ab initio nuclear structure:
Open-shell Sn isotopes via Bogoliubov coupled cluster theory

Workshop on Progress in Ab Initio Nuclear Theory - TRIUMF

Pepijn DEMOL

Supervisors Thomas Duguet
Riccardo Raabe

Co-supervisor Alexander Tichai

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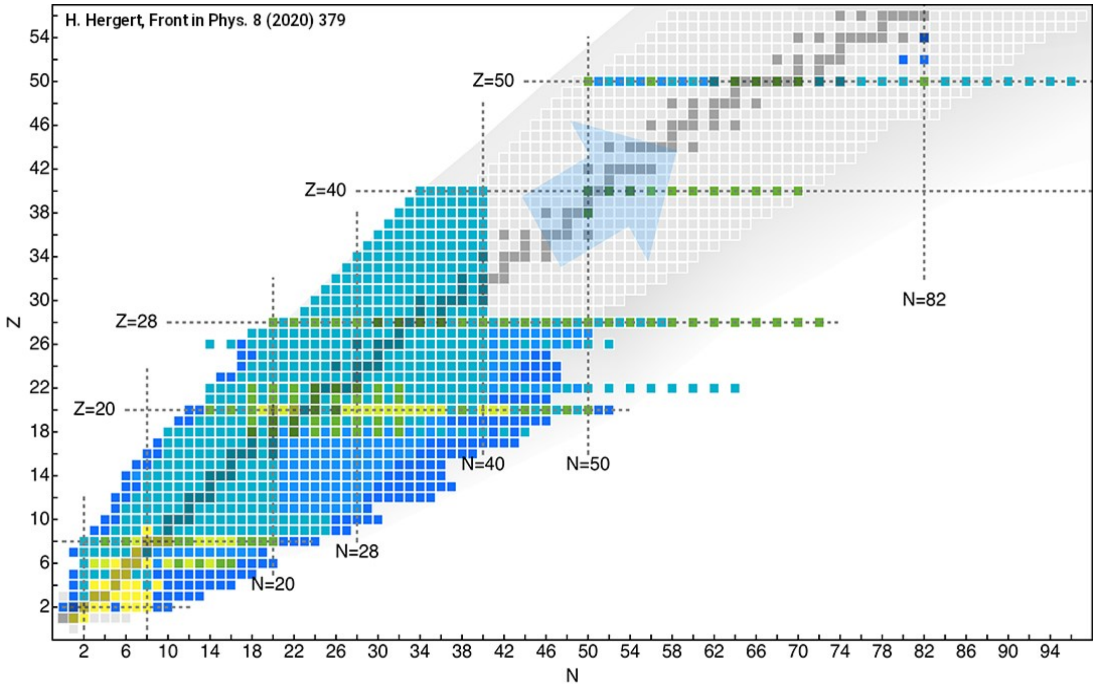
Open-shell frontier of ab initio many-body methods

- Open-shell nuclei
  - Vast majority
  - Strongly correlated
  - Spectroscopy at very frontier
- Push to heavier systems
  - **Polynomial** expansion methods required
- Single-refence symmetry-conserving approaches fail
  - Multi-reference techniques
  - Valence-space methods
  - **Symmetry-breaking approaches**
- Singly open-shell nuclei break particle-number symmetry
  - **Bogoliubov quasi-particle** framework
  - Grand canonical potential $\Omega \equiv H - \lambda A$



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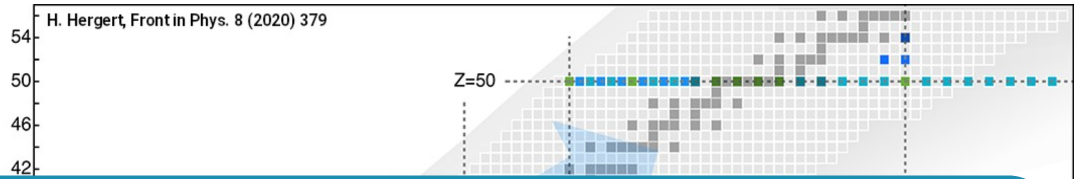
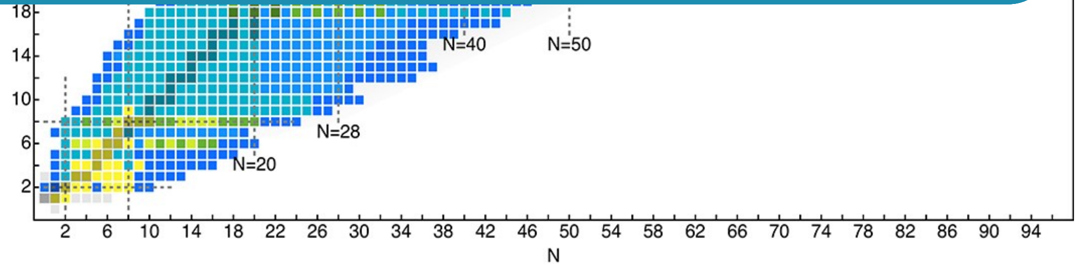


Equation-of-motion Bogoliubov coupled cluster (EOM-BCC)

= **non-perturbative** correlation expansion method for ground and **excited states** of **singly open-shell** nuclei



  - Valence-space methods
  - **Symmetry-breaking approaches**
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Bogoliubov coupled cluster (BCC)

- BCC extends standard CC to singly open-shell nuclei [1]
- **Exponential Ansatz** $|\Psi_0^A\rangle = e^{\mathcal{T}}|\Phi\rangle$

  where $\mathcal{T} \equiv \frac{1}{2!}\sum_{k_1k_2} t_{k_1k_2}\beta^\dagger_{k_1}\beta^\dagger_{k_2} + \frac{1}{4!}\sum_{k_1k_2k_3k_4} t_{k_1k_2k_3k_4}\beta^\dagger_{k_1}\beta^\dagger_{k_2}\beta^\dagger_{k_3}\beta^\dagger_{k_4} + \cdots$
- Special care to **constrain** $\langle A\rangle$ *(details on poster)*

Quasi-particle creation operators

Unitary mix of single-particle creation and annihilation operators $\{c^\dagger_p, c_p\}$

$$\beta^\dagger_k = \sum_p U_{pk}c^\dagger_p + V_{pk}c_p$$

Excitation amplitudes

Solutions of a set of **non-linear algebraic equations** which must be **solved iteratively**

$$\left\langle \Phi^{k_1k_2k_3\cdots}\middle| \Omega\, e^{\mathcal{T}} \middle|\Phi\right\rangle_C = 0$$

- In practice, truncate to **single** and **doubles** excitations (BCCSD) $\mathcal{T} \approx \mathcal{T}_1 + \mathcal{T}_2$
- Recently implemented in spherical (**J-scheme**) formulation
  - Non-trivial **angular-momentum-coupling** automated by `AMC` [2]

➔ **Immense speed up & reduction in storage cost**

[1] A. Signoracci et al., Phys. Rev. C 91, 064320 (2015)
[2] A. Tichai et al., Eur. Phys. J. A 56 10 272 (2020)

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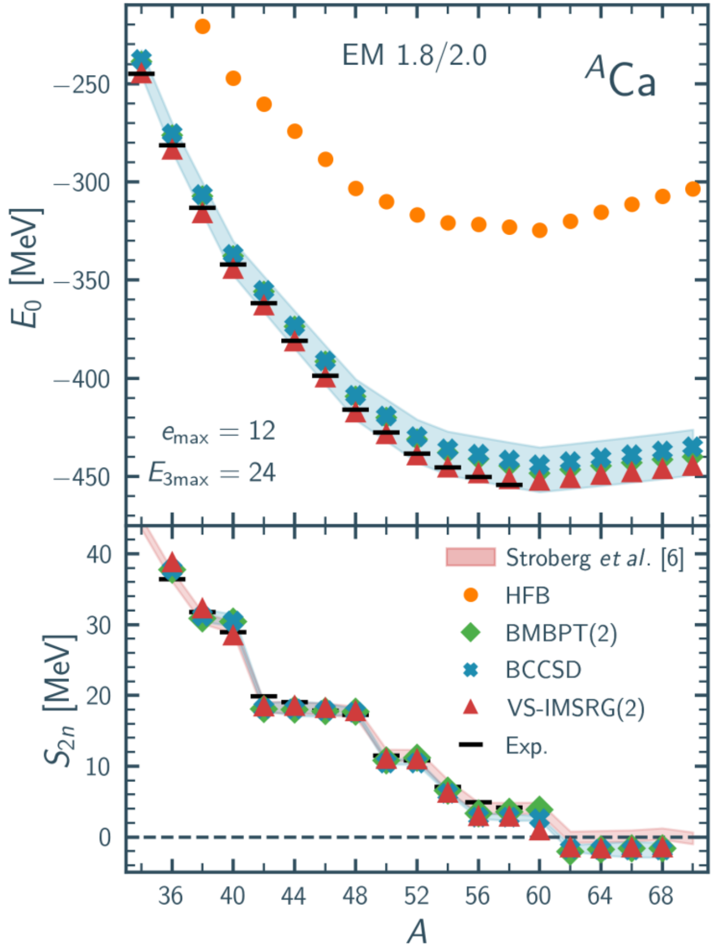
BCC benchmark against VS-IMSRG

A. Tichai, PD, T. Duguet, Phys. Lett. B (submitted), [arXiv:2307.15619]



- BCCSD benchmark against VS-IMSRG(2) in Ca chain
- BCCSD error band built from estimated many-body uncertainties

Take away

- Agreement withing uncertainties
- Consistent dripline prediction

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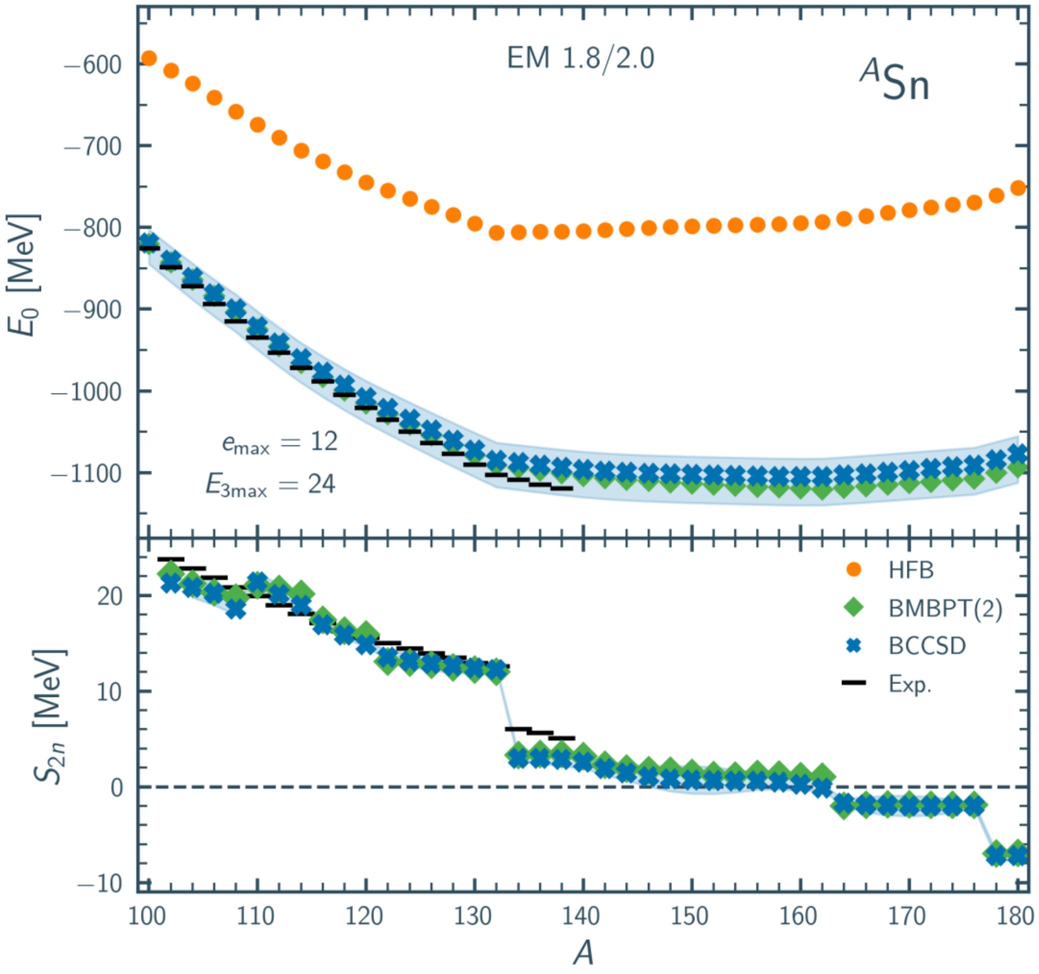
Heavy-mass BCCSD calculations



- BCCSD for heavy tin isotopes: ^{100}Sn – ^{180}Sn

Take away

- Shown to be scalable up to ^{180}Sn
- Flat trend in S_{2n} impedes drip line prediction
- Ongoing effort to reduce uncertainty
  - Implementation of leading-order triple excitations
  - Push basis size: natural orbitals + IT

A. Tichai, PD, T. Duguet, Phys. Lett. B (submitted), [arXiv:2307.15619]

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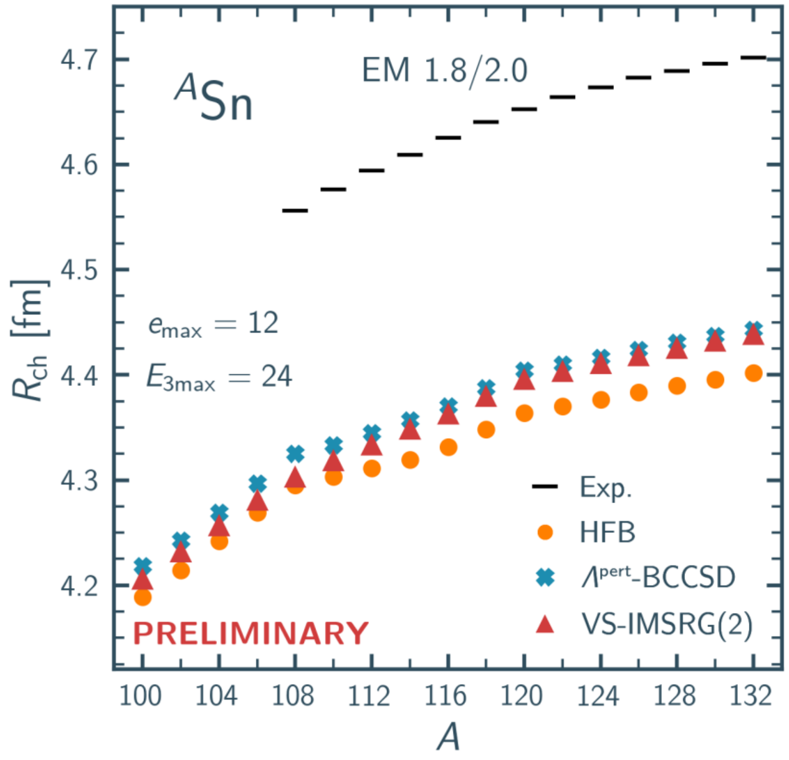
Extension to nuclear charge radii



- Evaluation of nuclear **charge radii**

Take away

- Good agreement with VS-IMSRG
- Distance to experiment known deficiency of EM1.8/2.0 interaction
- Future studies
  - Investigate kinks at shell closures
  - Skin thickness study in heavy tins

A. Tichai, PD, T. Duguet, Phys. Lett. B (submitted), [arXiv:2307.15619]

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Summary

- Computationally efficient CC formulation applicable to open-shell nuclei
- J-scheme implementation shown to be scalable up to heavy tin isotopes
- Once combined with equation-of-motion techniques

➔ **Spectroscopy of heavy singly open-shell nuclei from first principles**

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Collaboration

CEA:

T. Duguet
B. Bally
J. P. Ebran
M. Frosini
A. Roux
A. Scalesi
V. Somà
G. Stellin
L. Zurek

KU Leuven:

U. Vernik

Technische Universität Darmstadt:

A. Tichai
R. Roth

Oak Ridge National Laboratory:

G. Hagen

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Many-body uncertainty

$$\epsilon \equiv \epsilon_{\text{FBS}} + \epsilon_{\text{3NB}} + \epsilon_{\text{PNO2B}} + \epsilon_{\text{CC}} + \epsilon_{\text{PNR}}$$

		in Sn
ϵ_{FBS}	finite basis size (e_{max})	$\sim$ 2% of E
ϵ_{3NB}	three-body truncation ($E_{3\text{max}}$)	$\sim$ 0.4 MeV
ϵ_{PNO2B}	particle-number-conserving normal-ordered 2B	$\sim$ 2% of E
ϵ_{CC}	CC wavefunction truncation (BCCSD)	$\sim$ 8% of E_{corr} (attractive)
ϵ_{PNR}	lacking particle-number-restoration	$\sim$ 0.3 MeV

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Towards heavy-mass *ab initio* nuclear structure:

Open-shell Sn isotopes via Bogoliubov coupled cluster theory

Pepijn DEMOL [1], Alexander TICHAI [2], Thomas DUGUET [1,3]

1: KU Leuven, Instituut voor Kern- en Stralingsfysica, 3001 Leuven, Belgium
2: Institut für Kernphysik, Technische Universität Darmstadt, 64289 Darmstadt, Germany
3: IRFU, CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France

Open-shell frontier of *ab initio* many-body methods

H. Hergert, Front in Phys. 8 (2020) 379

- Open-shell nuclei
  - **Vast majority**
  - Strongly correlated
- Existing methods target mostly ground state
  - **Open-shell spectroscopy** at very frontier
  - Polynomial expansion methods required
- Single-reference symmetry-conserving approaches fail
  - Multi-reference techniques
  - Valence-space methods
  - **Symmetry-breaking approaches**
- Singly open-shell nuclei break particle-number symmetry
  - Bogoliubov quasi-particle framework

➔ **Equation-of-motion Bogoliubov coupled cluster (EOM-BCC)**

Quasi-particle formalism

- Quasi-particle operators defined via unitary **Bogoliubov transformation**

$$\beta_k = \sum_p U^*_{pk} c_p + V^*_{pk} c^\dagger_p$$

- Corresponding vacuum serves as the **reference state** $|\Phi\rangle \equiv C \prod_k \beta_k |0\rangle$
- **Grand potential operator** Ω expressed in quasi-particle basis

$$\Omega \equiv H - \lambda A = \Omega^{00} + \Omega^{20} + \Omega^{11} + \Omega^{02} + \Omega^{40} + \Omega^{31} + \cdots + \Omega^{60} + \cdots$$

where e.g. $$\Omega^{31} \equiv \frac{1}{3!\,1!} \sum_{k_1k_2k_3k_4} \Omega^{31}_{k_1k_2k_3k_4} \beta^\dagger_{k_1}\beta^\dagger_{k_2}\beta^\dagger_{k_3}\beta_{k_4}$$

Bogoliubov coupled cluster (BCC)

- BCC extends standard CC to singly open-shell nuclei [1]
- **Exponential Ansatz** $|\Psi^A_0\rangle = e^{\mathcal{T}}|\Phi\rangle$

where $\mathcal{T} \equiv \frac{1}{2!}\sum_{k_1k_2} t_{k_1k_2}\beta^\dagger_{k_1}\beta^\dagger_{k_2} + \frac{1}{4!}\sum_{k_1k_2k_3k_4} t_{k_1k_2k_3k_4}\beta^\dagger_{k_1}\beta^\dagger_{k_2}\beta^\dagger_{k_3}\beta^\dagger_{k_4} + \cdots$

- BCCSD: truncate to **single** and **double** excitations $\mathcal{T} \approx \mathcal{T}_1 + \mathcal{T}_2$
- Non-Hermitian **similarity-transformed** grand potential operator $\tilde{\Omega} \equiv e^{-\mathcal{T}}\,\Omega\, e^{\mathcal{T}}$
- Ground-state energy $\Omega_0 = \langle \Phi | \tilde{\Omega} | \Phi \rangle = \langle \Phi | \Omega\, e^{\mathcal{T}} | \Phi \rangle_C$
- Unknown $t_{k_1k_2k_3\cdots}$ obtained from set of algebraic equations $\langle \Phi^{k_1k_2k_3\cdots} | \Omega\, e^{\mathcal{T}} | \Phi \rangle_C = 0$

➔ Coupled non-linear equations solved **iteratively** $\mathcal{T}^{(i+1)}_N \equiv \mathcal{T}^{(i)}_N + \mathcal{R}^{(i)}_N(\Omega)$

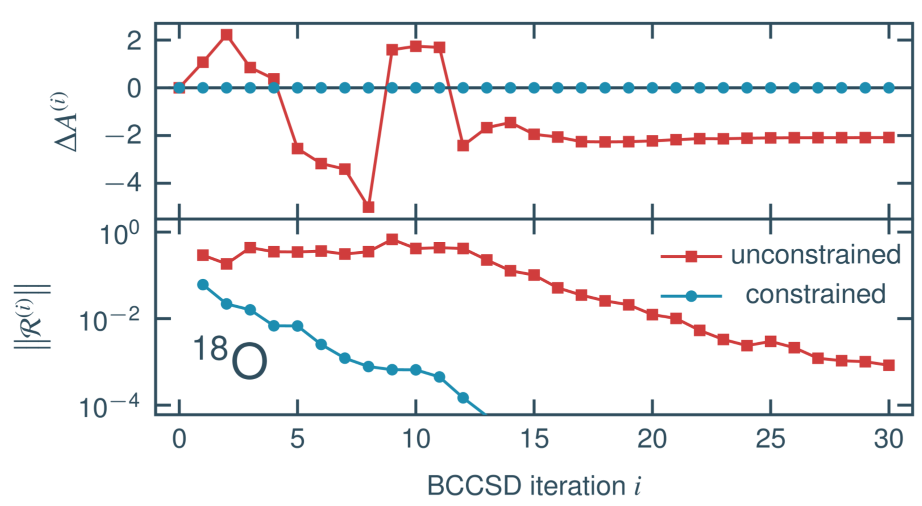
Computational aspects

- **J-scheme** formulation: exploit spherical symmetry of Ω, $|\Phi\rangle$ and quasi-particle basis

➔ Non-trivial angular-momentum-coupling automated by AMC [2]

- Convergence accelerated using **mixing:** direct inversion of iterative subspace
- **Constrain** $\langle A \rangle$ by updating $\Omega^{(i)} \equiv H - \lambda^{(i)} A$ at each BCC iteration

➔ $\lambda^{(i)}$ determined from $\Delta A^{(i+1)} = \langle \Phi | A\,(\mathcal{T}^{(i)}_1 + \mathcal{R}_1(H)) | \Phi \rangle_c - \lambda^{(i)} \langle \Phi | A\, \mathcal{R}_1(A) | \Phi \rangle_c = 0$

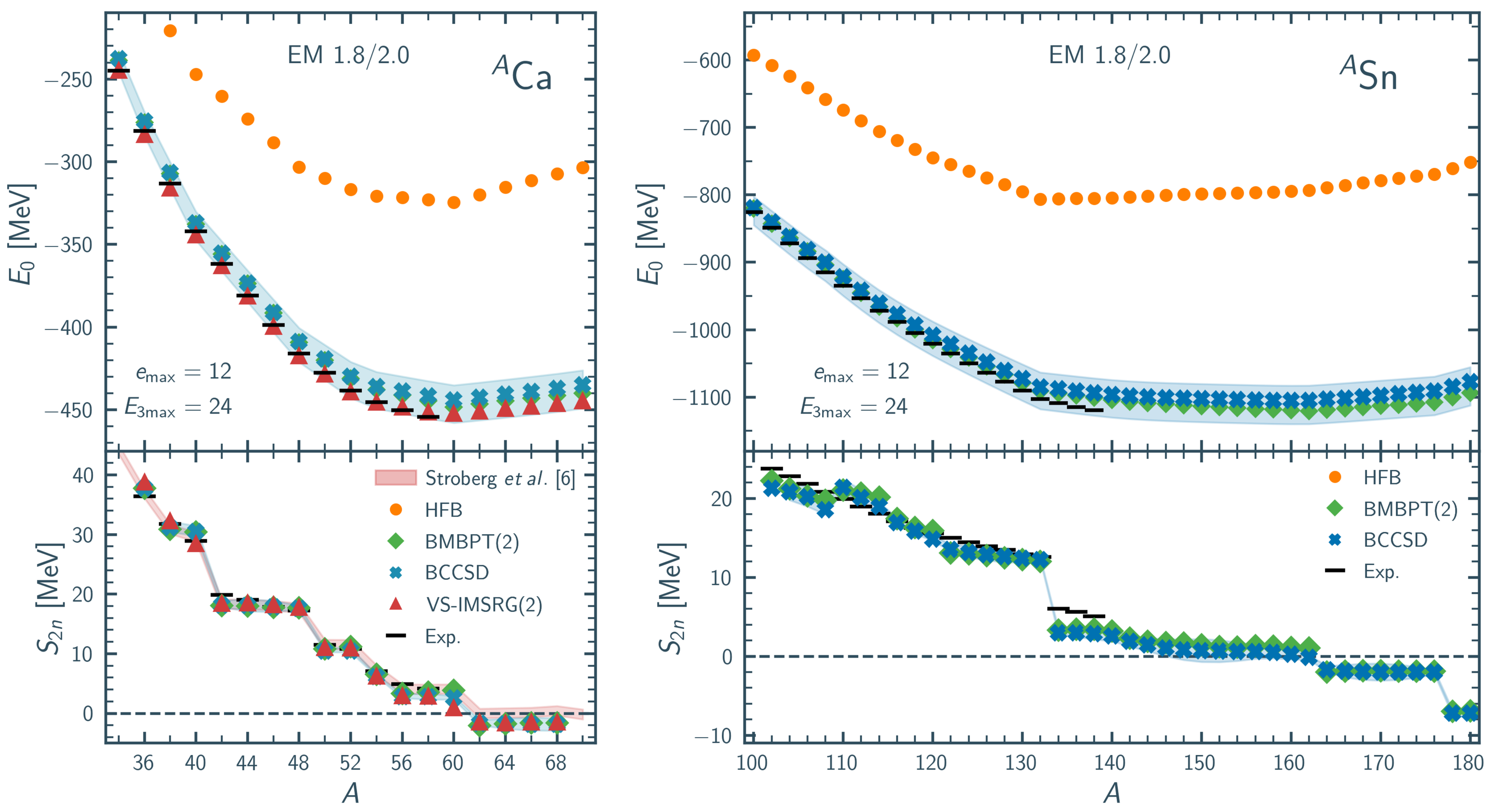


Outcomes

- $\langle A \rangle$ constrained at each iteration
- Computationally cheap
- Overall convergence accelerated
- Applicable to BMBPT [3]

Heavy-mass BCC calculations

- Total **ground-state binding energy** along **calcium** and **tin** chain comparing [4]
  - Hartree-Fock-Bogoliubov (HFB)
  - Bogoliubov many-body perturbation theory (BMBPT(2)) [5]
  - Valence-space in-medium similarity renormalization group (VS-IMSRG(2)) [6]
  - **BCCSD**
- NN + 3N forces derived from chiral EFT: EM 1.8/2.0 [7]
- 3N matrix elements stored using reduced NO2B format [8]



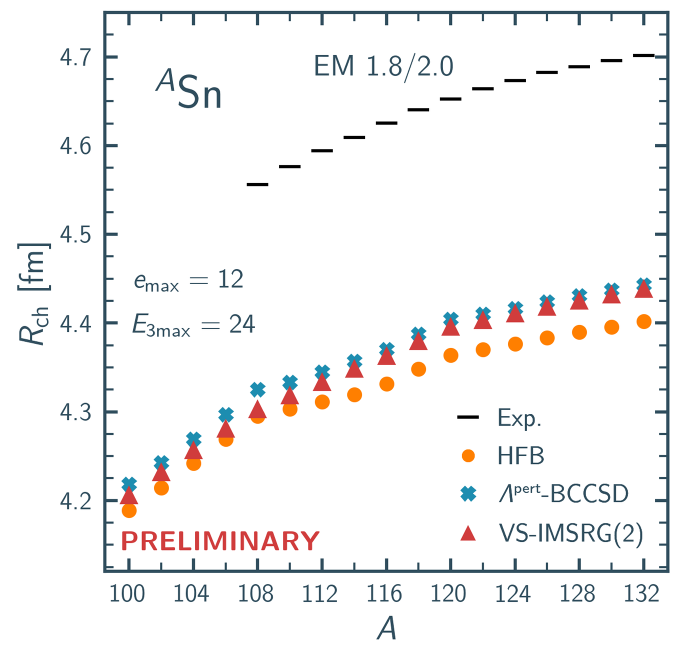
- BCCSD agrees with VS-IMSRG within uncertainties
- Perturbative BMBPT performs well thanks to softness of EM 1.8/2.0 interaction
- Error band built from ad hoc estimation of many-body uncertainties: **finite basis** + 3-body basis + normal-ordered 2-body + **CC truncation** + particle-number restoration

Extension to nuclear charge radii

- Evaluation of *rms* **charge radii**

➔ via perturbative Λ-BCCSD, where $\Lambda \approx \mathcal{T}^\dagger$

- Good agreement with VS-IMSRG(2)
- Distance to experiment attributable to interaction
- Non-negligible impact of dynamical correlations
- Easily extendable to neutron-rich tin isotopes



Future study

- First-principle predictions of differential charge radii across N=82 shell closure

Conclusion and outlook

Conclusion

- Computationally efficient CC formulation applicable to open-shell nuclei
- Effective particle-number constraint in BCC, applicable to BMBPT
- First-time implementation of BCCSD in symmetry-restricted J-scheme form
- Shown to be scalable up to heavy tin isotopes

Outlook

- Ongoing implementation of leading-order triples corrections for improved accuracy
- Description of excited states from equation-of-motion techniques
- Reduced basis size, natural orbitals + IT, to improve precision for heavy nuclei
- Implementation of electromagnetic observables to perform spectroscopy
- Generation of *ab initio* pseudo-data to constrain future EDF parametrizations

➔ **Spectroscopy of heavy singly open-shell nuclei from first principles**

[1] A. Signoracci et al., Phys. Rev. C 91, 064320 (2015)
[2] A. Tichai et al., Eur. Phys. J. A 56 10 272 (2020)
[3] P. Demol, A. Tichai, T. Duguet, in preparation (2024)
[4] A. Tichai, P. Demol, T. Duguet, submitted (2024) [arXiv:2307:15619]
[5] A. Tichai et al., Phys. Lett. B 786 195–200 (2018)
[6] R. S. Stroberg et al., Phys. Rev. Lett. 126, 022501 (2021)
[7] K. Hebeler et al., Phys. Rev. C 83, 031301(R) (2011)
[8] T. Miyagi et al., Phys. Rev. C 105(1), 014302 (2022)